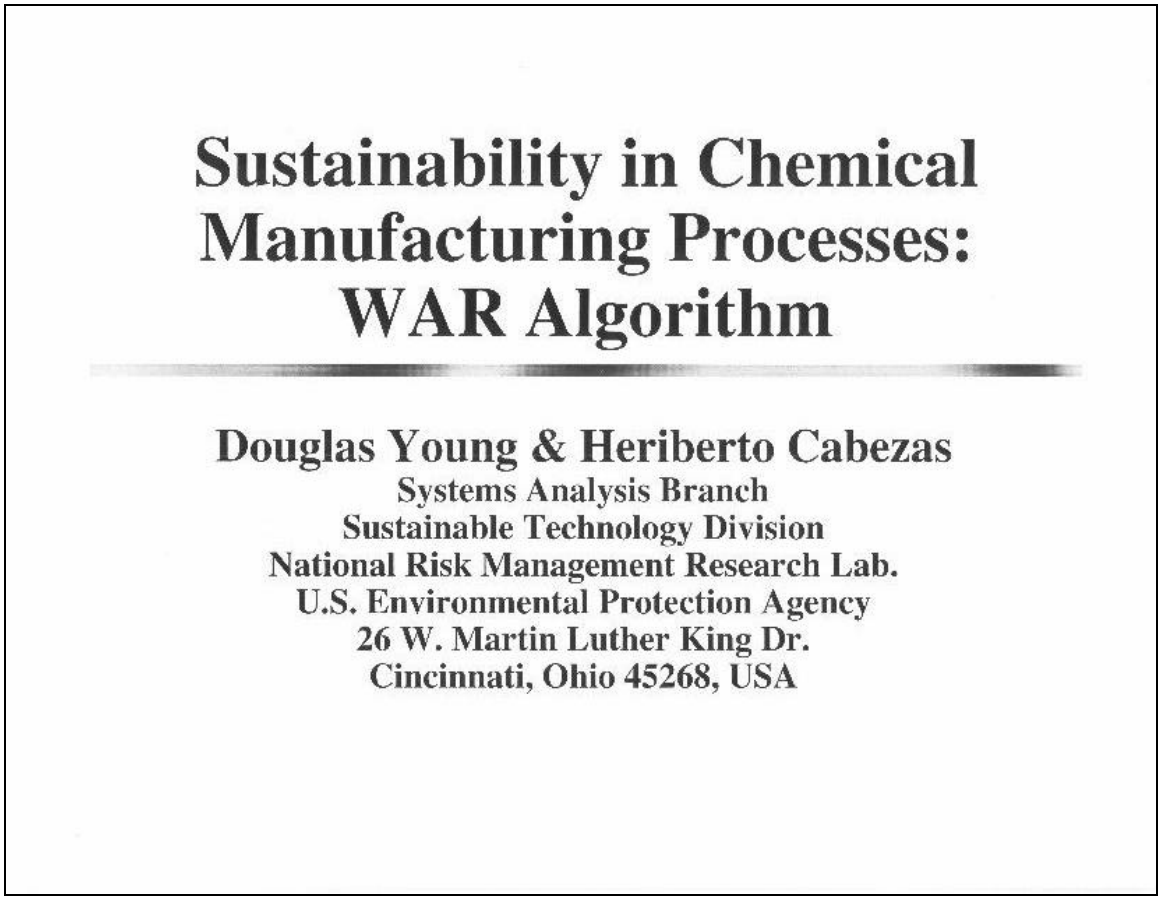
Sustainability in Chemical Manufacturing Processes: The Waste Reduction (WAR) Algorithm

Abstract

The WAste Reduction (WAR) algorithm has been developed and implemented into the ChemCad™ chemical process simulator. The algorithm is a method for combining a variety of industry defined environmental impacts (*e.g.,* global warming potential, ozone depletion potential, human toxicity, *etc.*) into pollution indices. These pollution indices (*e.g.*, pollution generation index and pollution output index) represent impact values of the waste generated in a process and not simply the amount of waste generated in a process. The method is inherently flexible which allows the user to emphasize or de-emphasize the individual impact categories in the calculation of the pollution indices to address their specific needs. These indices can be used to design or re-design chemical processes to be more environmentally friendly. A case study will be presented which uses the WAR algorithm to re-design a typical chemical process. The case study will present the affects of applying emphasis to different impact categories. The case study will also examine the different types of information that can be obtained from the different pollution indices. These aspects then will be united to create a more environmentally friendly chemical process.

Slide Presentation



Current Collaborators

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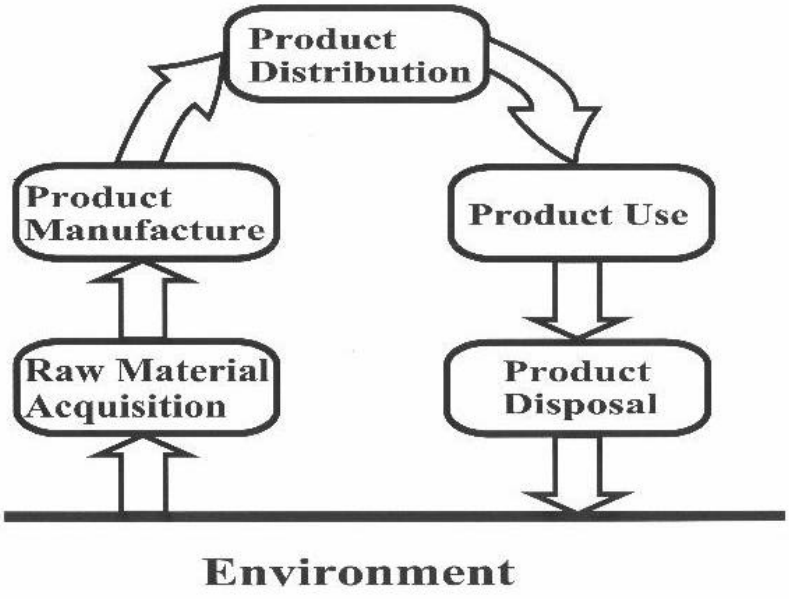
Product Life-Cycle



What is Potential Environmental Impact?

***Potential Environmental Impact** is the **unrealized** effect or impact that the emission of material and/or energy would have the environment on average.*

Conservation Equation
(Over Product Life Cycle)

$$\frac{dI_{syst}}{dt} = \dot{I}_{in} - \dot{I}_{out} + \dot{I}_{gen}$$

$$\begin{bmatrix}\textit{Impact}\\ \textit{Accumulation}\end{bmatrix} = \begin{bmatrix}\textit{Impact}\\ \textit{Input}\end{bmatrix} - \begin{bmatrix}\textit{Impact}\\ \textit{Output}\end{bmatrix} + \begin{bmatrix}\textit{Impact}\\ \textit{Generation}\end{bmatrix}$$

$$0 = \dot{I}_{in} - \dot{I}_{out} + \dot{I}_{gen}$$

Sustainable Processes
(Over Product Life Cycle)

$$\dot{I}_{gen} = 0 \longrightarrow \infty \textit{ Sustainable}$$

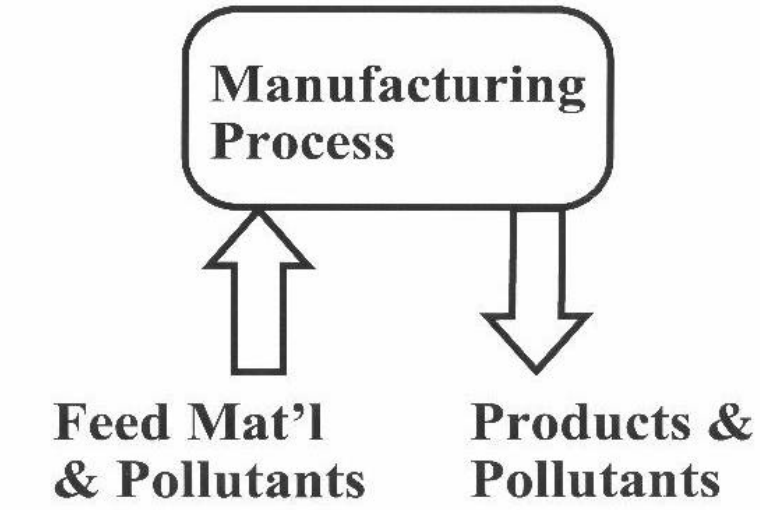
This is an idealized process which will not by its operation create new potential environmental impacts that do not already exist.

Real Processes
(Over Product Life Cycle)

$\dot{I}_{gen} > 0$ *for Real Processes*

Potential environmental impact will always be generated over the life cycle of a product.

Manufacturing Processes: WAR Algorithm



Conservation Equation
(Over Manufacturing Process)

$$\frac{dI_{syst}}{dt} = \dot{I}_{in} - \dot{I}_{out} + \dot{I}_{gen}$$

$$\begin{bmatrix}\textit{Impact}\\ \textit{Accumulation}\end{bmatrix} = \begin{bmatrix}\textit{Impact}\\ \textit{Input}\end{bmatrix} - \begin{bmatrix}\textit{Impact}\\ \textit{Output}\end{bmatrix} + \begin{bmatrix}\textit{Impact}\\ \textit{Generation}\end{bmatrix}$$

$$0 = \dot{I}_{in} - \dot{I}_{out} + \dot{I}_{gen}$$

Impact Generation Indexes

$$\dot{I}_{gen} = \frac{Impact\ \ Generated}{Hour}$$

$$\hat{I}_{gen} = \frac{\dot{I}_{out} - \dot{I}_{in}}{\dot{P}_{out}}$$

Impact Output Indexes

$$\dot{I}_{out} = \frac{Impact\ \ Output}{Hour}$$

$$\hat{I}_{out} = \frac{\dot{I}_{out}}{\dot{P}_{out}}$$

Chemical Processes

$$\dot{I}_{out} = \sum_{j}^{Streams} \sum_{i}^{Comps} x_{ij}\psi_i + \ldots$$

$$\dot{I}_{in} = \sum_{j}^{Streams} \sum_{i}^{Comps} F_j x_{ij}\psi_i + \ldots$$

Chemical Environmental Impact Function

$$\psi_i = \sum_{l}^{ImpCat} \alpha_l \psi_{il}^{s} + \ldots$$

α_l = ***relative weighting factor for impact l***

$\psi_{i\,l}^{s}$ = ***specific impact of chemical i for impact l***

Chemical Score Normalization

$$\psi_{ij}^{s} = \frac{Score_{ij}}{\langle (Score)_i \rangle_j}$$

ψ_{ij}^{s} = *Normalized score of chemical i for impact type j*

$Score_{ij}$ = *Raw score of chemical i for impact type j*

$\langle Score \rangle_j$ = *Arithmetic average of all scores for impact type j*

σ_j = *Standard deviation of all scores for impact type j*

Impact Categories

- Ozone Depletion Potential
- Global Warming Potential
- Smog Formation Potential
- Acidification Potential
- Human Toxicity by Ingestion Potential
- Human Toxicity by Inhalation/Dermal Exposure Potential
- Aquatic Toxicity Potential
- Terrestrial Toxicity Potential

Current Status

- Release ChemCad early 1999 (Chemstations)
- CRADA almost finished with Simulation Science
- Discussing CRADA with ASPEN TECH

Represents over 90% of process simulator market